Joachim Rang

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Informatikbericht Nr. 2014-05

Institute of Scientific Computing
Carl-Friedrich-Gauss-Fakultät
Technische Universität Braunschweig

Braunschweig, Germany

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This document was created July 2014 using $\LaTeX\,2_\varepsilon$.

Institute of Scientific Computing
Technische Universität Braunschweig
Hans-Sommer-Straße 65
D-38106 Braunschweig, Germany

url: www.wire.tu-bs.de
mail: wire@tu-bs.de

e-print: http://www.digibib.tu-bs.de/?docid=00057194

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The Prothero and Robinson example: Convergence studies for Runge–Kutta and Rosenbrock–Wanner methods

Joachim Rang

Institute of Scientific Computing, TU Braunschweig
j.rang@tu-bs.de

Abstract

It is well-known that one-step methods have order reduction if they are applied on stiff ODEs such as the example of Prothero–Robinson. In this paper we analyse the local error of Runge–Kutta and Rosenbrock–Wanner methods. We derive new order conditions and define B_{PR}-consistency. We show that for strongly A-stable methods B_{PR}-consistency implies B_{PR}-convergence. Finally we analyse methods from literature, derive new B_{PR}-consistent methods and present numerical examples. This analysis shows that Runge–Kutta methods and Rosenbrock–Wanner methods which are not stiffly accurate and are only consistent converge with order 2 in the stiff case, but the error constant may be large. As an improvement stiffly accurate methods can be considered, since the numerical error is now smaller, but the method converges only with order 1. The numerical results and the order of convergence can be improved if the derived order conditions are satisfied.

Keywords: example of Prothero–Robinson, order reduction, B-convergence, Runge–Kutta methods, Rosenbrock–Wanner methods, ODEs

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1 Introduction

In the simulation of stiff ODEs and differential algebraic equations (DAEs), Runge–Kutta (RK) and Rosenbrock–Wanner (ROW) methods seem to be a good choice since these classes of methods include A-stable schemes. A-stability guarantees in general a stable numerical solution. One disadvantage of one-step methods is the order reduction phenomenon for stiff problems such as the example of Prothero and Robinson [17]. For fully implicit Runge–Kutta methods like Gauß–Legendre methods the numerical order of convergence decreases from $2s$ to s, where s is the number of internal stages.

Order reduction can be observed for other stiff ODEs, too, such as semi-discretised parabolic PDEs, often called MOL-ODEs. Analytical results are proven by Ostermann and Roche [15]. They show that implicit Runge–Kutta methods may have a fractional order of convergence. Similar results are presented for Rosenbrock–Wanner methods in [16].

For Runge–Kutta methods Frank, Schneid and Ueberhuber in [6] introduced the concept of B-consistency and B-convergence. They show that B-consistency and B-stability imply B-convergence [7]. In contrast to the estimates for non-stiff problems the local and the global error in the case of stiff problems depend on a one-sided Lipschitz constant, and not on the classical Lipschitz constant. In several papers B-convergence of implicit Runge–Kutta methods is studied. For an overview we refer to [8] and [9].

In contrast to implicit Runge–Kutta methods Rosenbrock–Wanner methods can not be B-stable (see [9, 18] and the references cited in there). Scholz introduces B-consistency for Rosenbrock–Wanner methods [24] and proves that strongly A-stable Rosenbrock–Wanner methods are B-convergent if they are B-consistent. Moreover, order conditions are presented such that B-consistent Rosenbrock–Wanner methods can be developed. A Rosenbrock–Wanner method satisfying these order conditions from Scholz is the RODASP method from Steinebach [26].

More or less all error bounds which can be found in literature estimate the local or global error w.r.t. powers of the step-size. It is well-known that, for example, stiffly accurate Runge–Kutta methods such as Radau-IIA methods the local and global error can be estimated with τ^q/z in the case of the stiff Prothero–Robinson example. Here τ denotes the step-size and $z := \tau\lambda$, where λ is the given stiffness. The factor τ^q/z implies a numerical order of convergence of order $q-1$. Since z is very large for very stiff problems these error terms are often smaller than the error terms of order τ^q.

In this paper we introduce the concept of B_{PR}-consistency and B_{PR}-convergence similar to the concept of B-consistency and B-convergence from [6]. The only difference to [6] is that we concentrate only on the ex-

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ample of Prothero and Robinson. The aim of this paper is the analysis and the understanding of the convergence behaviour of implicit Runge–Kutta and Rosenbrock–Wanner methods. We prove that B_{PR}-consistent one-step methods of order q, which are A-stable with $R(\infty) < 1$, are B_{PR}-convergent of order q. A similar result for Rosenbrock–Wanner methods is presented from Scholz in [24], but his error constant depends on the step-size which has the effect that the convergence order is too large.

In Section 3 we consider implicit Runge–Kutta methods with a regular coefficient matrix and present new order conditions such that the methods can be B_{PR}-consistent of order q. These new order conditions are different from the ones for the non-stiff case. Only the condition for order one is needed in the stiff case. We show that Runge–Kutta methods with a regular coefficient matrix which are not stiffly accurate and which are only consistent converge with order 2 in the stiff case but the numerical error is large. It could be reduced if the methods are stiffly accurate. Now the numerical error is smaller but the method converges only with order 1. Our representation of the local error leads to a second kind of order conditions, which are related to the simplifying condition $C(q)$ (see also the analysis from Hairer and Wanner [9]). In this case convergence order q can be reached. In this paper we develop a new singly diagonally implicit Runge–Kutta (SDIRK) method which is B_{PR}-consistent of order 2, although the stage order of SDIRK methods can only be one.

In Subsection 4.2 we compare the numerical results with the analytical ones from Section 4.1. In the paper of Nørsett and Thomson [14] B-stable singly diagonally implicit Runge–Kutta (SDIRK) methods are considered. The convergence order is 2 for the stiff Prothero–Robinson example, but as stated above the error constant is large so that the numerical results are more worse than the results of a stiffly accurate SDIRK method although it converges only with order 1.

In Section 4 we analyse Rosenbrock–Wanner methods and derive new order conditions such that these methods are B_{PR}-consistent of order q. We analyse existing methods from literature in Section 4.1. For example in the paper of Scholz [24] several B_{PR}-consistent Rosenbrock–Wanner methods are presented. In the case of Rosenbrock–Wanner methods the same observations as for Runge–Kutta methods can be made. Rosenbrock–Wanner methods which are not stiffly accurate and are only consistent converge with order 2 in the stiff case, but again the error constant may be large. Again, as an improvement we consider stiffly accurate methods and the numerical error is now smaller, but the method converges only with order 1. Our representation of the local error leads to a second kind of order conditions (as in the case

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of Runge–Kutta methods) such that convergence order q can be reached. In Sections 6.2 and 6.5 we compare the numerical results for 2nd and 3rd order methods with the analytical ones from Section 6.1 and 6.3.

Finally we summarise the results of the paper and give an outlook to future investigations.

2 B_{PR}-consistency and B_{PR}-convergence

2.1 The example of Prothero–Robinson

We start our considerations with the well-known example of Prothero and Robinson (see [17]), which is given by

$$\dot{u} = \lambda(u - \varphi(t)) + \dot{\varphi}(t), \quad u(0) = \varphi(0), \quad \lambda \ll 0, \tag{1}$$

where $u(t) = \varphi(t)$ is the exact solution of (1). One-step methods have usually difficulties to solve this problem because they often have order reduction if λ is very small, i.e. the ODE is very stiff.

In the book of Hairer and Wanner [9] an analysis of the local error for Runge–Kutta methods applied on the ODE (1) can be found which shows that the convergence order decreases from the convergence order p to the stage order q. Therefore, several papers deal with this phenomenon and try to improve Runge–Kutta methods such that a better convergence order can be obtained. For an overview we refer to the book of Hairer and Wanner [9] or to the book of Strehmel and Weiner [27].

In this paper we make a careful analysis of the local error so that we are able to understand the behaviour of different Runge–Kutta and Rosenbrock–Wanner methods. Moreover, we are interested in developing new order conditions which give us the possibility to increase the convergence order when we solve the stiff Prothero–Robinson example or other stiff ODEs and DAEs. Therefore, we want to adapt the idea of Frank, Schneid and Ueberhuber who introduce the concept of B-consistency and B-convergence [6]. Since we are interested in a rigorous analysis of the Prothero–Robinson example we restrict ourselves to this problem.

2.2 B_{PR}-consistency

Let us apply a one-step method on the example of Prothero and Robinson and let $z := \tau\lambda$. For non-stiff problems we have $\tau \to 0$ and $z \to 0$, and the local error can be computed in the usual way, where the Lipschitz condition L of the rhs of the ODE is used. In the case of $\lambda \to -\infty$ in equation (1) we

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get a stiff problem and we have the situation that $\tau \to 0$ and simultaneously $z \to \infty$. For the time discretisation schemes considered in this paper the local error can be written in the form

$$\epsilon(t_{m+1}) = R(z)(u_m - \varphi(t_m)) + \delta_\tau(t_m), \tag{2}$$

where $R(z)$ is the stability function of the one-step method and $\delta_\tau(t_m)$ is an expansion of the local error in terms of τ^k/z^l. Note that for the local error the first term is always zero since it is assumed that the exact solution is known at time t_m. Consistency can now be defined in the following way:

Definition 2.1. *A one-step method is called B_{PR}-consistent of order $\bar{q}$ if the local discretisation error for the Prothero–Robinson example satisfies the inequality*

$$\epsilon(t) \leq C_1 \tau^{\bar{q}} + C_2 \frac{\tau^{\bar{q}+1}}{|z|}, \tag{3}$$

where the non-negative constants C_1 and C_2 are independent of the step-size τ and the stiffness λ.

As the analysis of the Prothero–Robinson example in the book of Hairer and Wanner [9] shows the local error of L-stable Runge–Kutta methods is given by $\mathcal{O}(\tau^{\bar{q}+1}/z)$. Therefore, we have included the second term $\tau^{\bar{q}+1}/|z|$ in Definition 2.1.

2.3 B_{PR}-convergence

Next we want to study the global error of a one-step method which is applied to the example of Prothero and Robinson. Therefore, we apply the representation of the local error (equation (2)) to get a formula in dependency of t_0. We have

$$\begin{aligned}
\epsilon(t_{m+1}) &= R(z)(u_m - \varphi(t_m)) + \delta_\tau(t_m) \\
&= R(z)^2(u_{m-1} - \varphi(t_{m-1})) + R(z)\delta_\tau(t_{m-1}) + \delta_\tau(t_m) = \cdots = \\
&= R(z)^{m+1}(u_0 - \varphi(t_0)) + \sum_{j=0}^{m} R(z)^{m-j}\delta_\tau(t_j).
\end{aligned}$$

The first term vanishes since the initial condition is valid. Next we define convergence in the stiff case as follows:

Definition 2.2. *A one-step method is called B_{PR}-convergent of order $\bar{q}$ if the global error satisfies*

$$\epsilon(t_m) \leq C_1 \tau^{\bar{q}} + C_2 \frac{\tau^{\bar{q}+1}}{|z|},$$

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where C_1 and C_2 are non-negative constants which are independent of the step-size τ and the stiffness λ.

Next we show that B_{PR}-consistency and A-stability imply B_{PR}-convergence or, to be more precise, that B_{PR}-consistency of order $\bar{q}$ and A-stability imply B_{PR}-convergence of order $\bar{q}-1$. If the one-step method is A-stable with $R(\infty)=0$ the converge order in the stiff case is $\bar{q}$, too, if equidistant time-steps are used.

Theorem 2.3. *Consider an A-stable one-step method with $R(\infty)\leq 1$. Assume that the local error can be written in the form (2) and that the one-step method is B_{PR}-consistent of order $\bar{q}+1$.*

- *Then the one-step method is B_{PR}-convergent of order $\bar{q}$.*
- *If $R(\infty)<0$ then for constant step-sizes τ the one-step method is B_{PR}-convergent of order $\bar{q}+1$.*
- *If $R(\infty)=0$ the one-step method is B_{PR}-convergent of order $\bar{q}+1$.*

Proof. This theorem can be proven in an analogous way as in the case of implicit Runge–Kutta methods (see [9]). We start with an A-stable one-step method and let $\rho=R(\infty)$. Then the global error reads as

$$\epsilon(t_{m+1})=\sum_{j=0}^{m}\rho^{m-j}\delta_\tau(t_j).$$

Since $|\rho|\leq 1$ we have

$$|\epsilon(t_{m+1})|\leq\sum_{j=0}^{m}|\delta_\tau(t_j)|\leq(m+1)\max_{j=0,\ldots,m}|\delta_\tau(t_j)|. \tag{4}$$

Next the quantity $\delta_\tau(t_j)$ can be estimated with the help of inequality (3). Since $m=(t_m-t_0)/\tau$ we finally have

$$|\epsilon(t_{m+1})|\leq(t_m-t_0)\left(C_1\tau^{\bar{q}}+C_2\frac{\tau^{\bar{q}+1}}{z}\right)$$

and we have proven the first statement.

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If $\rho < 0$ we can improve our last estimate if constant step-sizes τ are used. In this case we have

$$\begin{aligned}\epsilon(t_{m+1}) &= \sum_{j=0}^{m}\left[\rho^{m-j} \pm \sum_{k=0}^{m-j-1}\rho^k\right]\delta_\tau(t_j)\\ &= \sum_{k=0}^{m}\rho^k\delta_\tau(t_0) + \sum_{j=1}^{m}\sum_{k=0}^{m-j}\rho^k(\delta_\tau(t_j)-\delta_\tau(t_{j-1})).\end{aligned}$$

With

$$\sum_{k=0}^{m}\rho^k = \frac{1-\rho^{m+1}}{1-\rho}$$

it follows

$$\epsilon(t_{m+1}) = \frac{1-\rho^{m+1}}{1-\rho}\delta_\tau(t_0) + \sum_{j=1}^{m}\frac{1-\rho^{m-j+1}}{1-\rho}(\delta_\tau(t_j)-\delta_\tau(t_{j-1})).$$

Since

$$\delta_\tau(t_j)-\delta_\tau(t_{j-1}) = \tau\dot{\delta}_\tau(t_{j-1}) + \mathcal{O}(\tau^2)$$

we finally get

$$\delta_\tau(t_{m+1}) \le C_1\tau^{\bar{q}+1} + C_2\frac{\tau^{\bar{q}+2}}{z}$$

and have proven the second statement. In the case of an L-stable method the global error reads as

$$\epsilon(t_{m+1}) = \delta_\tau(t_m),$$

i.e. the global error is equal to the local one. □

The estimate (4) is not sharp, but we are only interested in an estimate w.r.t. to potentials of τ. As in the paper of Scholz [24] the geometrical series can be applied, but that technique has the only effect that the error constants are smaller.

3 Runge–Kutta methods

3.1 Application to ODEs

We start our considerations with an initial value problem of the form

$$\dot{\boldsymbol{u}} = \boldsymbol{F}(t,\boldsymbol{u}), \quad \boldsymbol{u}(0) = \boldsymbol{u}_0. \tag{5}$$

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A Runge–Kutta (RK) method with s internal stages [9, 27] is a one–step–method for solving (5) of the form

$$\boldsymbol{k}_i = \boldsymbol{F}\left(t_m + \alpha_i \tau_m, \boldsymbol{u}_m + \tau_m \sum_{j=1}^{s} a_{ij} \boldsymbol{k}_j\right), \quad i = 1, \ldots, s, \tag{6}$$

$$\boldsymbol{u}_{m+1} = \boldsymbol{u}_m + \tau_m \sum_{i=1}^{s} b_i \boldsymbol{k}_i. \tag{7}$$

Coefficients of the Runge–Kutta method are a_{ij}, b_i and c_i and should be chosen in such a way that some order conditions are satisfied to obtain a sufficient high consistency order. In the following we assume that the coefficient matrix $\mathbf{A} = (a_{ij})_{i,j=1}^{s}$ is regular. For example fully implicit Runge–Kutta methods like Radau-IIA methods or diagonally implicit Runge–Kutta methods without an explicit first stage are met this condition.

If we apply a Runge–Kutta method on the problem of Dahlquist [3], i.e. on $\dot{u} = \lambda u$ with $\lambda \in \mathbb{C}$ and $\operatorname{Re} \lambda < 0$, the stability function of the Runge–Kutta method $R(z)$, $z := \lambda\tau$ can be computed. The stability function is given by

$$R(z) = 1 + z\boldsymbol{b}(I - z\mathbf{A})^{-1}\boldsymbol{e},$$

where $\boldsymbol{e} := (1, \ldots, 1)^\top \in \mathbb{R}^s$, $\boldsymbol{b} := (b_1, \ldots, b_s)^\top$ and $\mathbf{A} := (a_{ij})_{i,j=1}^{s}$. The Runge–Kutta method is called A-stable if $|R(z)| \leq 1$ for all $z \in \mathbb{C}^-$. If, furthermore, $R(\infty) < 1$ the Runge–Kutta method is called strongly A-stable and L-stable if $R(\infty) = 0$ (see [4]).

The property A-stability implies that a Runge–Kutta method is dissipative for Dahlquist's problem. But what happens if non-linear problems are solved? For this case B-stability may be important. Runge–Kutta methods are B-stable if they are algebraically stable, i.e. if the matrices

$$\mathbf{B} = \operatorname{diag}(b_1, \ldots, b_s) \quad \text{and} \quad \mathbf{M} = \mathbf{BA} + \mathbf{A}^\top\mathbf{B} - \boldsymbol{b}\boldsymbol{b}^\top$$

are positive semi-definite. For example the Gauß-Legendre, the Radau-IA, the Radau-IIA, and the Lobatto-IIIC methods are algebraically stable.

3.2 Local error

Next we apply the Runge–Kutta method (6)–(7) on the example of Prothero and Robinson, i.e. on equation (1). First we get

$$k_i = \lambda\left(u_m + \tau \sum_{j=1}^{s} a_{ij} k_j - \varphi(t_m + c_i\tau)\right) + \dot{\varphi}(t_m + c_i\tau).$$

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In the following we use the abbreviations

$$\varphi_i^{(k)} := \varphi^{(k)}(t_m + \alpha_i\tau), \quad i = 1, \dots, s, \quad \varphi_m^{(k)} := \varphi^{(k)}(t_m), \quad k \geq 0,$$
$$\mathbf{\Phi}^{(k)} := (\varphi_1^{(k)}, \dots, \varphi_s^{(k)})^\top, \quad \boldsymbol{k} := (k_1, \dots, k_s)^\top, \quad \boldsymbol{c} := (c_1, \dots, c_s)^\top.$$

It follows

$$k_i = \lambda \left(u_m + \tau \sum_{j=1}^{s} a_{ij}k_j - \varphi_i \right) + \dot{\varphi}_i.$$

Using the vector notation introduced above we obtain

$$\boldsymbol{k} = \lambda(u_m\boldsymbol{e} + \tau\mathbf{A}\boldsymbol{k} - \mathbf{\Phi}) + \dot{\mathbf{\Phi}}$$

and

$$\boldsymbol{k} = (I - z\mathbf{A})^{-1}(\lambda u_m\boldsymbol{e} - \lambda\mathbf{\Phi} + \dot{\mathbf{\Phi}}), \tag{8}$$

where $z := \lambda\tau$. Inserting (8) into (7) yields

$$u_{m+1} = u_m + \tau\boldsymbol{b}^\top(I - z\mathbf{A})^{-1}[\lambda(u_m\boldsymbol{e} - \mathbf{\Phi}) + \dot{\mathbf{\Phi}}. \tag{9}$$

In the non-stiff case we have $\tau \to 0$ and $z := \tau\lambda \to 0$. Here we are interested in the stiff case, i.e. $\tau \to 0$ and simultaneously $z \to -\infty$. A convergence result can be found in the book of Hairer and Wanner [9] , but they use the simplifying conditions $B(p)$ and $C(q)$, which are introduced by Butcher in [1] and given by

$$\begin{aligned}
B(p): \quad & \sum_{i=1}^{s} b_i c_i^{k-1} &&= 1/k, && k = 1, \dots, p, \\
C(q): \quad & \sum_{j=1}^{s} a_{ij} c_j^{k-1} &&= c_i^k/k, && i = 1, \dots, s, k = 1, \dots, q.
\end{aligned}$$

The coefficient of a singly diagonally implicit Runge–Kutta (SDIRK) method is a lower triangular matrix which is regular and the coefficients of the main diagonal are all equal to γ. These methods can only satisfy the simplifying condition $C(1)$ and these classes of methods converge in general only with order 1 or 2 in the case of the stiff Prothero–Robinson example. Therefore, we look for a more precise representation of the local error. Such a representation can be found in [21], too, and is stated in the next theorem.

Theorem 3.1. *Consider the Runge–Kutta method (6)–(7) with a regular coefficient matrix* $\mathbf{A}$*. Then the local error of a Runge–Kutta method applied to the stiff Prothero–Robinson example (1) can be represented as*

$$\epsilon(t_{m+1}) = R(z)(u_m - \varphi(t_m)) + \delta_\tau(t_m), \tag{10}$$

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where

$$\delta_\tau(t_m) = \sum_{k=2}^{p} \left[\boldsymbol{b}^\top \mathbf{A}^{-1}\boldsymbol{c}^k - 1\right] \varphi_m^{(k)} \frac{\tau^k}{k!} + \mathcal{O}(\tau^{p+1})$$

$$+ \sum_{k=2}^{\infty} \boldsymbol{b}^\top \mathbf{A}^{-l} \sum_{l=1}^{k-1} \left\{ \mathbf{A}^{-1}\boldsymbol{c}^{k-l} \frac{1}{(k-l)} - \boldsymbol{c}^{k-l-1} \right\} \cdot \varphi_m^{(k-l)} \frac{\tau^{k-l}}{(k-l-1)!z^l}. \quad (11)$$

Proof. see [21]. □

In [21] only the term δ_τ is considered since a convergence analysis was omitted. In contrast to [21] in equation (11) we sum to ∞ to omit problems with the remainder, since they depend on terms of the form τ^k/z^l. These remainder look strange on the first view, but we know from stiffly accurate Runge–Kutta methods that they converge with order $\mathcal{O}(\tau^{p+1}/z)$. From the representation of the local error, i.e. equation (11), we get new order conditions

$$\boldsymbol{b}^\top \mathbf{A}^{-1}\boldsymbol{c}^k = 1, \quad k = 2, \ldots, \bar{q}, \quad (12)$$

$$\boldsymbol{b}^\top \mathbf{A}^{-(l+1)} \frac{1}{k-l} \boldsymbol{c}^{k-l} = \boldsymbol{b}^\top \mathbf{A}^{-l}\boldsymbol{c}^{k-l-1}, \quad (13)$$

for $l = \max\{1, k-\bar{q}\}, \ldots, k-1$ and $k = 1, \ldots, \infty$. With the help of these order conditions we can formulate the next result.

Theorem 3.2. *The Runge–Kutta method (6)–(7) is B_{PR}-consistent of order $\bar{q}$ if condition (12) is satisfied for $k = 2, \ldots, \bar{q}$ and (13) for $k = 2, \ldots, \infty$ and $l = \max\{1, k-\bar{q}\}, \ldots, k-2$.*

As the above analysis shows it is important to consider the terms τ^k/z^l since the local error of stiffly accurate methods is of order τ^2/z, i.e. these methods converge only with order 1. In the next step we look how these conditions can be satisfied. For fully implicit Runge–Kutta methods there is a relationship between the simplifying conditions $B(p)$ and $C(q)$ and our new order conditions (12) and (13).

Theorem 3.3. *Let a Runge–Kutta method with a regular coefficient matrix A be given which satisfies the simplifying conditions $B(1), \ldots, B(q)$ and $C(1), \ldots, C(q)$.*

- *Then the order condition (12) is satisfied for all $k = 1, \ldots, q$.*
- *Then the order condition (13) is satisfied for all $k = 2, \ldots, \infty$ and all $l = \max\{1, k-q\}, \ldots, k-1$.*

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Proof. First we note that the simplifying condition $C(k)$ can be written as $\mathbf{A}^{-1}\boldsymbol{c}^k = k\boldsymbol{c}^{k-1}$ for $k = 1, \ldots, q$.

- We have
$$\boldsymbol{b}^\top \mathbf{A}^{-1}\boldsymbol{c}^k = k\boldsymbol{b}^\top \boldsymbol{c}^{k-1} = 1$$
because the simplifying condition $B(k)$ is valid for $k = 1, \ldots, q$.

- Since the simplifying condition $C(\tilde{q})$ is valid for $k - l = \tilde{q}$ and $\tilde{q} \in \{1, \ldots, q\}$ condition (22) can be written as
$$\mathbf{A}^{-(l+1)}\frac{1}{k-l}\boldsymbol{c}^{k-l} = \mathbf{A}^{-l}\boldsymbol{c}^{k-l-1}.$$

□

From this result it follows that a Runge–Kutta method with stage order q is at least B_{PR}-consistent of order q.

A Runge–Kutta method is called *stiffly accurate* if $a_{si} = b_i$ for $i = 1, \ldots, s$ and $c_s = 1$ hold. Note that condition (12) is automatically satisfied if the Runge–Kutta method is stiffly accurate. In this case the local error is equal to the global one and given by $\mathcal{O}(\tau^q/z)$. In this case the simplifying conditions $B(2), \ldots, B(p)$ may not be needed to fulfil the order condition (13).

4 Results for SDIRK methods

4.1 Convergence analysis

We start our considerations with two classes of fully implicit Runge–Kutta methods. First we mention the Radau-IIA methods, which are stiffly accurate and satisfy the simplifying conditions $C(1), \ldots, C(s)$. Therefore, the local error is given by $\mathcal{O}(\tau^{s+1}/z)$. Moreover, Radau-IIA methods are L-stable. Therefore, the global error is equal to the local one.

Next we consider the Gauß-Legendre methods which satisfy the simplifying conditions $B(1), \ldots, B(2p)$ and $C(1), \ldots, C(s)$. The local error is dominated by the first term in the representation (11) and it is given by $\mathcal{O}(\tau^{s+1})$. Since $R(\infty) = \pm 1$ the local error is given by $\mathcal{O}(\tau^s)$. This estimate can be improved for odd s and constant step-sizes (see Theorem 2.3).

Next we want to study singly diagonally implicit Runge–Kutta (SDIRK) methods. First we consider methods with two internal stages, which form the Butcher table

$$\begin{array}{c|cc} \gamma & \gamma & 0 \\ c_2 & c_2 - \gamma & \gamma \\ \hline & 1 - b_2 & b_2 \end{array}.$$

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First we consider a stiffly accurate method, i.e. $b_2 = \gamma$ and $c_2 = 1$. The remaining coefficient γ is determined with the help of the simplifying condition $B(2)$ to guarantee second order accuracy (see [5, 9]). In our numerical experiments this method is denoted by SDIRK2. Since the method is stiffly accurate the new condition (12) is fulfilled for all positive k. Since the condition (13) is not satisfied, the local and the global error are of order $\mathcal{O}(\tau^2/z)$.

In the book of Strehmel and Weiner [27] the coefficients in the above Butcher table are chosen such that the method is of order 3, i.e. the coefficients of the method are given by

$$b_2 = \frac{1-2\gamma}{2(c_2-\gamma)}, \qquad c_2 = 1-\gamma, \qquad \gamma = \frac{1}{2} + \frac{1}{6}\sqrt{3}.$$

We call this method SDIRK2B, since with this setting the method is L- and B-stable, but none of the conditions (12) and (13) are fulfilled. Therefore, the local and the global error are of order $\mathcal{O}(\tau^2)$.

In the paper of Nørsett and Thomson [14] B-stable SDIRK methods are developed. We study a third order method [14, Equation (5.4)] called SDIRK3B in this paper with the Butcher table

$$\begin{array}{c|ccc}
5/6 & 5/6 & 0 & 0 \\
29/108 & -61/108 & 5/6 & 0 \\
1/6 & -23/183 & -33/61 & 5/6 \\
\hline
 & 26/61 & 324/671 & 1/11
\end{array}.$$

As in the case of the SDIRK2B method the local and the global error are of order $\mathcal{O}(\tau^2)$.

Next we introduce a new L-stable SDIRK method which is only consistent, but satisfies the new condition (12) for $k = 2$. This method is called SDIRK13PR and we take three internal stages, therefore we set $a_{32} = 1/2$, $\gamma = 2/3$, $c_2 = 6/5$ and $c_3 = 3/4$. The other coefficients are computed and given by $b_2 = 121/108$ and $b_3 = 32/27$. The local and global error are of order $\mathcal{O}(\tau^3) + \mathcal{O}(\tau^2/z)$. Which factor is larger depends on the problem and on the step-size τ. We come back to this problem later in Section 4.2.

Our next method is the 4th order SDIRK4 method from Hairer and Wanner [9, Table 6.5]. This method is stiffly accurate, but no further order conditions are satisfied. The coefficients are presented in the following Butcher

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table:

$$\begin{array}{c|ccccc}
1/4 & 1/4 & 0 & 0 & 0 & 0 \\
3/4 & 1/2 & 1/4 & 0 & 0 & 0 \\
11/20 & 17/50 & -1/25 & 1/4 & 0 & 0 \\
1/2 & 371/1360 & -137/2720 & 15/544 & 1/4 & 0 \\
1 & 25/24 & -49/48 & 125/16 & -85/12 & 1/4 \\
\hline
 & 25/24 & -49/48 & 125/16 & -85/12 & 1/4
\end{array}.$$

Since the method is stiffly accurate the local and the global error are of order $\mathcal{O}(\tau^2/z)$.

Cameron, Palmroth and Piche introduce in [2] the *quasi stage order* for improving the convergence behaviour of stiff ODEs and DAEs. An SDIRK method which has quasi stage order 2 is given by the Butcher table [2, Formula (16)]

$$\begin{array}{c|cccc}
1/4 & 1/4 & 0 & 0 & 0 \\
11/28 & 1/7 & 1/4 & 0 & 0 \\
1/3 & 61/144 & -49/144 & 1/4 & 0 \\
1 & 0 & 0 & 3/4 & 1/4 \\
\hline
 & 0 & 0 & 3/4 & 1/4
\end{array}.$$

In our numerical experiments we call this method SDIRK2CPP. Since the method is stiffly accurate the new condition (12) is satisfied for all positive k. Moreover, the condition (13) is fulfilled for $k = 3$ and $l = 1$. Since the condition (13) for $k = 4$ and $l = 2$ is not valid, the method is not B_{PR}-consistent of order 2 and the local and global error are of order $\mathcal{O}(\tau^3/z) + \mathcal{O}(\tau^2/z^2)$. It depends now on the problem which error term is dominated. If $\lambda \to -\infty$ the term $\mathcal{O}(\tau^3/z)$ is dominant. For medium stiff problems the error depends on $\mathcal{O}(\tau^2/z^2)$, which leads in practise to a very poor convergence behaviour, i.e. the numerical error does not change for certain τ.

In [20] the SDIRK2PR method is created. This method has three internal stages and is of order 2 and stiffly accurate. The coefficients are summarised in Table 1. Although the SDIRK2PR method fulfills condition (13) for $k = 3$ and $l = 1$, this method can not be B_{PR}-consistent of order 2 as the next Lemma shows. Therefore, the local error is given by $\mathcal{O}(\tau^2/z^2) + \mathcal{O}(\tau^3/z)$.

Lemma 4.1. *A stiffly accurate SDIRK method of order 2 with $a_{11} \neq 0$ and with three internal stages can not be B_{PR}-consistent of order 2.*

Proof. The order condition (13) for $k = 3$ and $l = 1$ reads as

$$\gamma b_2 c_2 - 3\gamma^2 + \gamma^3 - b_2 c_2^2 + \gamma = 0. \tag{14}$$

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Table 1: Set of coefficients for the SDIRK2PR method

γ	$=$	$2.3728621957824146e-01$			
a_{21}	$=$	$7.6271378042175854e-01$	c_1	$=$	$2.3728621957824146e-01$
a_{31}	$=$	$6.5555390873299095e-01$	c_2	$=$	$1.0000000000000000e+00$
a_{32}	$=$	$1.0715987168876759e-01$	c_3	$=$	$1.0000000000000000e+00$
b_1	$=$	$6.5555390873299095e-01$	$\hat{b}_1$	$=$	$7.6271378042175854e-01$
b_2	$=$	$1.0715987168876759e-01$	$\hat{b}_2$	$=$	$2.3728621957824146e-01$
b_3	$=$	$2.3728621957824146e-01$	$\hat{b}_3$	$=$	$0.0000000000000000e+00$

For the case $k = 4$ and $l = 2$ we have

$$-3\gamma b_2 c_2 + 2\gamma^2 + b_2\gamma^2 + b_2 c_2^2 - \gamma = 0. \tag{15}$$

With the help of the order condition $B(2)$ we can compute b_2, which is given by

$$b_2 = \frac{1 - 4\gamma + 2\gamma^2}{2(c_2 - \gamma)}.$$

Then we can resolve equation (14) w.r.t. c_2 and get

$$c_2 = 2\gamma \frac{\gamma^2 + 1 - 3\gamma}{1 - 4\gamma + 2\gamma^2}.$$

Next we insert b_2 and c_2 into equation (15) and obtain the quadratic equation

$$1 - 4\gamma + 2\gamma^2 = 0,$$

which is the dominator of c_2. Therefore, our non-linear system is not solvable. □

Next we create a stiffly accurate B_{PR}-consistent method of order 2. We know that we need 4 internal stages. As free parameters we choose $c_2 = 1/2$ and $c_3 = 1$. The remaining coefficients can be computed by solving a non-linear systems of equations. The coefficients of the new method SDIRK2PR2 are presented in Table 2.

Let us now summarise our theoretical results about the local and global errors of Runge–Kutta methods with a regular coefficient matrix A. A consistent method has the local error $\mathcal{O}(\tau^2)$ if no further order conditions are

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Table 2: Set of coefficients for the SDIRK2PR2 method

a_{21}	$=$	$2.071067811865475e-01$	a_{22}	$=$	$2.928932188134525e-01$
a_{31}	$=$	$7.071067811865476e-01$	a_{32}	$=$	$0.000000000000000e+00$
a_{33}	$=$	$2.928932188134525e-01$	a_{41}	$=$	$1.121320343559643e+00$
a_{42}	$=$	$-5.857864376269050e-01$	a_{43}	$=$	$1.715728752538099e-01$
a_{44}	$=$	$2.928932188134525e-01$			
b_1	$=$	$1.121320343559643e+00$	$\hat{b}_1$	$=$	$7.071067811865476e-01$
b_2	$=$	$-5.857864376269050e-01$	$\hat{b}_2$	$=$	$0.000000000000000e+00$
b_3	$=$	$1.715728752538099e-01$	$\hat{b}_3$	$=$	$2.928932188134525e-01$
b_4	$=$	$2.928932188134525e-01$	$\hat{b}_4$	$=$	$0.000000000000000e+00$

satisfied and the method is not stiffly accurate. In this case the method converges with order 2 in the stiff case. The disadvantage of this method is the relatively large error constant. This error constant can be reduced if the method is stiffly accurate. But in this case the local error would be $\mathcal{O}(\tau^2/z)$, i.e. the method converges only with order 1. This convergence behaviour can be improved if the method fulfils condition (13) for certain k and l. A summary of the properties of our discussed methods can be found in Table 3.

Table 3: Properties of selected RK methods

method	s	p	stiffly acc.	B-stab.	$k=2$	3	$k=3$ 1	4 2	5 3	4 1
SDIRK2	2	2	x	-	x	x	-	-	-	-
SDIRK2B	2	3	-	x	x	-	-	-	-	-
SDIRK3B	2	3	-	x	x	-	-	-	-	-
SDIRK13PR	3	1	-	-	x	x	-	-	-	-
SDIRK4	5	4	x	-	x	x	-	-	-	-
SDIRK3CPP	4	3	x	-	x	x	x	-	-	-
SDIRK2PR	3	2	x	-	x	x	x	-	-	-
SDIRK2PR2	4	2	x	-	x	x	x	x	x	-

4.2 Numerical results

Next we present some numerical results and consider the example of Prothero and Robinson [17] with $\varphi(t) = 10 - (10+t)\exp(-t)$. We solve this problem

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in the time interval $(0, 2]$ and take the discrete l_2-error. As step-sizes we use $\tau = 0.1 \cdot 2^{-l}$, where $l = 0, \ldots, 10$. The results for $\lambda = -10^5$ and $\lambda = -10^6$ are presented in Figure 1. Let us first consider the case $\lambda = -10^6$, i.e. the

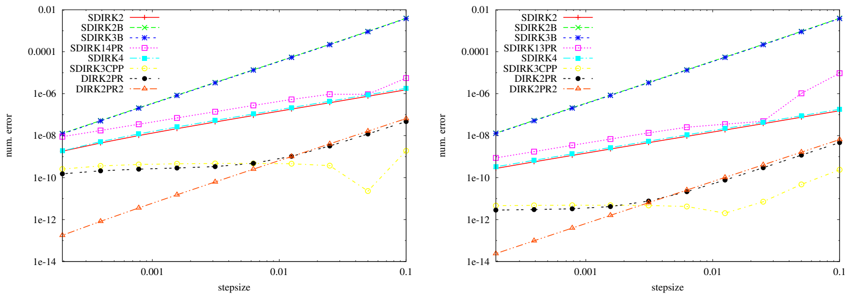

Figure 1: τ versus error for (1) with $\lambda = -10^5$ (left) and $\lambda = -10^6$ (right)

right visualisation in Figure 1. First we observe that the largest numerical errors are computed by the B-stable methods SDIRK2B and SDIRK3B, since they do not satisfy any of the order conditions (12) and (13). From the representation of the local error, i.e. equation (11), it can be concluded that the error term $\mathcal{O}(\tau^2)$ is larger than $\mathcal{O}(\tau^2/z)$. Therefore, these methods converge with order 2. The SDIRK13PR methods shows an interesting behaviour. For large τ the method converges with order 3, since the local error is dominated by $\mathcal{O}(\tau^3)$. If the step-size is smaller the error term $\mathcal{O}(\tau^2/z)$ becomes dominant and the numerical order of convergence decreases to one. The SDIRK2 and SDIRK4 methods are both stiffly accurate. Therefore, the numerical error is of order $\mathcal{O}(\tau^2/z)$. This is the reason why the numerical errors of the SDIRK13PR method and the stiffly accurate SDIRK methods SDIRK2 and SDIRK4 are similar for $\tau < 0.03$. The SDIRK2PR2 method converges with order 2 for all step-sizes, since it is B_{PR}-consistent of order 2. For large τ SDIRK2PR gives the same numerical results, but for smaller step-sizes the error term $\mathcal{O}(\tau^2/z^2)$ destroys the convergence. For smaller τ, i.e. $\tau \in [2 \cdot 10^{-5}, 0.003]$, no convergence at all can be observed, the numerical error is approximately 10^{-12}. The same problems for smaller step-sizes can be observed for the SDIRK3CPP method. Since the method satisfies the condition (13) for $k = 3$ and $l = 1$ we have order 3 for large time-steps.

Next we consider the case $\lambda = -10^5$. The results are shown in the left part of Figure 1, and it is obvious that the limiting $z \to \infty$ can not always be applied. For methods which do not satisfy any of our new conditions the results are more or less the same as for the case $\lambda = -10^6$. Therefore,

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we analyse only the other methods which satisfy at least one further condition. We start with the SDIRK13PR method. The factor z is now smaller in comparison to the previous test case. Therefore, the numerical error is dominated by $\mathcal{O}(\tau^2/z)$ and the numerical order of convergence is one. The SDIRK2PR and SDIRK2PR2 methods show the same behaviour as before, i.e. the SDIRK2PR2 method converges with order 2 for all step-sizes and the SDIRK2PR method with order 2 if τ is large, otherwise no convergence can be observed. The behaviour of the SDIRK3CPP method is very strange. There is no improvement of the results for smaller step-sizes. These numerical results show that the new order conditions must be satisfied for all $l = k - 2$ and $k = 3, \ldots, \infty$. Otherwise the numerical results for medium stiff problem are rather poor.

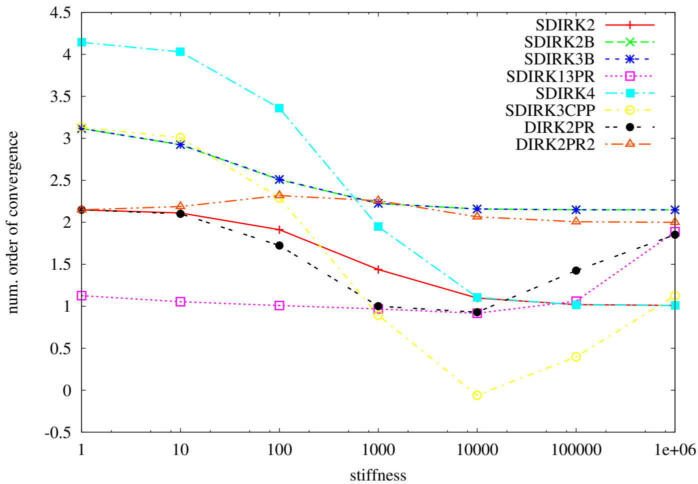

Figure 2: λ versus numerical order of convergence for (1)

In Figure 2 we plot the stiffness factor λ against the numerical order of convergence. Again we consider $\varphi(t) = 10 - (10 + t)\exp(-t)$ and solve this problem in the time interval $(0, 2]$. As step-size we use $\tau = 0.1 \cdot 2^{-l}$, where $l = 0, \ldots, 5$. From the discrete l_2-error the numerical order of convergence is computed and finally the mean convergence order is plotted in Figure 2.

Let us start with the SDIRK13PR method. It converges with order one for almost all values of λ. Only for $\lambda = -10^6$ the convergence order increases, since condition (12) is satisfied for $k = 2$. SDIRK2, SDIRK2PR and SDIRK2PR2 converge with order 2 for non-stiff problems. The converge or-

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der decreases to one for large values of $|\lambda|$ in the case of the SDIRK2 method. For the SDIRK2PR method it can be observed that the order decreases to 1, but only for medium stiff problems. Only the SDIRK2PR2 method converges for all values of λ with order 2.

The SDIRK2B and SDIRK3B methods converge with order 3 in the non-stiff case and then the order decreases to 2 if the problem becomes more stiff. The numerical order of convergence for the SDIRK3CPP method is 3 for non-stiff problems. Then the order decreases to zero for $\lambda = -10^4$, and then the order increases again for $\lambda = -10^6$. This "zero–convergence" can be observed, since the method does not satisfy condition (13) for $k = 4$ and $l = 2$. Therefore, in this case the local error is of order $\mathcal{O}(\tau^2/z^2)$. For the SDIRK4 method it can be observed that the numerical order of convergence decreases from 4 to 1.

Next we visualise the numerical error for very small step-sizes τ to show that for all methods the numerical error can be reduced to machine accuracy. We solve the Prothero–Robinson example with $\lambda = -10^6$ and use the step-sizes $\tau = 1/(100 \cdot 2^k)$ with $k = 0, \ldots, 11$. The results are plotted in

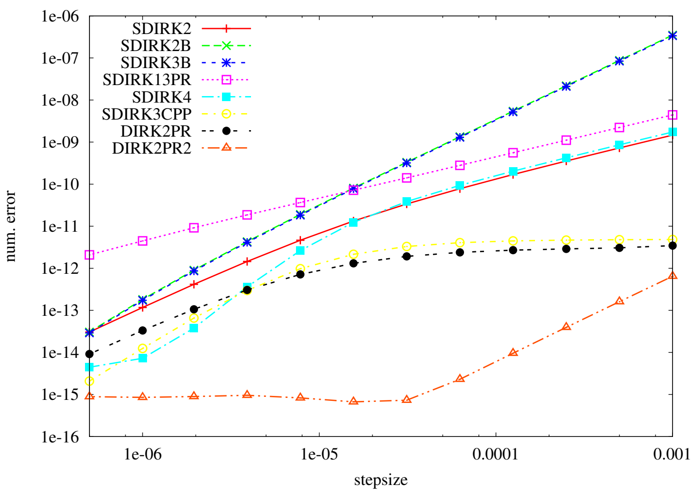

Figure 3: τ versus numerical error for (1)

Figure 3 and show that the analytical statements hold only for large $|z|$. The SDIRK13PR method converges with order 1, since τ is too small for a convergence of order 3 (see discussion above). SDIRK2B and SDIRK3B converge with order 2 for "larger" step-sizes, for smaller ones the order of convergence

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increases. A similar behaviour can be observed for the SDIRK2 and SDIRK4 method. Here the order of convergence increases from 1 to 2 and from 1 to 4, resp. The most interesting methods are SDIRK2PR and SDIRK3CPP. For "larger" step-sizes τ there can be observed almost no convergence. Only for step-sizes τ smaller than 10^{-4} an improvement of the numerical results is observed. Only the SDIRK2PR2 method converges with order 2 for all step-sizes, since the method is B_{PR}-consistent of order 2.

5 Rosenbrock–Wanner methods

5.1 The local error

A Rosenbrock–Wanner (ROW) method with s internal stages is given by

$$M\boldsymbol{k}_i = \boldsymbol{F}\left(t_m + \alpha_i\tau_m, \tilde{\boldsymbol{U}}_i\right) + \tau_m\mathbf{J}\sum_{j=1}^{i}\gamma_{ij}\boldsymbol{k}_j + \tau_m\gamma_i\dot{\mathbf{F}}(t_m, \mathbf{u}_m), \tag{16}$$

$$\tilde{\boldsymbol{U}}_i = \boldsymbol{u}_m + \tau_m\sum_{j=1}^{i-1}a_{ij}\boldsymbol{k}_j, \quad i = 1, \ldots, s,$$

$$\boldsymbol{u}_{m+1} = \boldsymbol{u}_m + \tau_m\sum_{i=1}^{s}b_i\boldsymbol{k}_i, \tag{17}$$

where $\mathbf{J} := \partial_{\boldsymbol{u}}\boldsymbol{F}(t_m, \boldsymbol{u}_m)$, α_{ij}, γ_{ij}, b_i are the parameters of the method,

$$\alpha_i := \sum_{j=1}^{i-1}\alpha_{ij}, \quad \gamma_i := \sum_{j=1}^{i-1}\gamma_{ij}, \quad \gamma := \gamma_{ii} > 0,\ i = 1, \ldots, s.$$

If the parameters α_{ij}, γ_{ij}, and b_i are chosen appropriately, a sufficient consistency order can be obtained. Additional consistency conditions arise if $\mathbf{J}$ is only an approximation to $\partial_{\boldsymbol{u}}\boldsymbol{F}(t_m, \boldsymbol{u}_m)$, or if $\mathbf{J}$ is an arbitrary matrix. This class of methods is called W–methods, [27]. If a ROW method is applied to a semidiscretised partial differential equation, further order conditions should be satisfied to avoid order reduction, see [13, 24, 21].

The ROW method (16)–(17) requires the successive solution of s linear systems of equations with the same matrix $\mathbf{I} - \gamma\tau_m\mathbf{J}$. The right hand side of the i–th linear system of equations depends on the solutions of the first to the $(i-1)$–st system. Thus, a main difference of ROW methods to implicit methods is that it is not necessary to solve a non-linear system of equations in each discrete time, but only a fixed number of linear systems of equations.

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Next we apply the Rosenbrock–Wanner method (16)–(17) on the Prothero–Robinson problem (1) and compute the numerical error. First we get

$$k_i = \lambda \left(u_m + \tau \sum_{j=1}^{i} \beta_{ij} k_j - \varphi(t_m + \alpha_i \tau) \right) \\ + \dot{\varphi}(t_m + \alpha_i \tau) + \tau \gamma_i (\ddot{\varphi}(t_m) - \lambda \dot{\varphi}(t_m)),$$

where $\beta_{ij} := \alpha_{ij} + \beta_{ij}$. To abbreviate we set

$$\begin{aligned} \varphi_i^{(k)} &:= \varphi^{(k)}(t_m + \alpha_i \tau), \quad i = 1, \ldots, s, \quad \varphi_m^{(k)} := \varphi^{(k)}(t_m), \quad k \geq 0, \\ \mathbf{\Phi}^{(k)} &:= (\varphi_1^{(k)}, \ldots, \varphi_s^{(k)})^\top, \quad \boldsymbol{k} := (k_1, \ldots, k_s)^\top, \quad \boldsymbol{e} := (1, \ldots, 1)^\top, \\ \boldsymbol{\alpha} &:= (\alpha_1, \ldots, \alpha_s)^\top, \quad \boldsymbol{\gamma} := (\gamma_1, \ldots, \gamma_s)^\top, \\ \boldsymbol{b} &:= (b_1, \ldots, b_s)^\top, \quad \mathbf{B} := (\beta_{ij})_{i,j=1}^{s}. \end{aligned}$$

It follows

$$k_i = \lambda \left(u_m + \tau \sum_{j=1}^{i} \beta_{ij} k_j - \varphi_i \right) + \dot{\varphi}_i + \tau \gamma_i (-\lambda \dot{\varphi}_m + \ddot{\varphi}_m).$$

Using the vector notation introduced above we obtain

$$\boldsymbol{k} = \lambda (u_m \boldsymbol{e} + \tau \mathbf{B} \boldsymbol{k} - \mathbf{\Phi}) + \dot{\mathbf{\Phi}} + \tau \boldsymbol{\gamma} (\ddot{\varphi}_m - \lambda \dot{\varphi}_m)$$

and

$$\boldsymbol{k} = (I - z\mathbf{B})^{-1} (\lambda u_m \boldsymbol{e} - \lambda \mathbf{\Phi} + \dot{\mathbf{\Phi}} + \tau \boldsymbol{\gamma} (\ddot{\varphi}_m - \lambda \dot{\varphi}_m)), \tag{18}$$

where $z := \lambda \tau$. Inserting (18) into (17) yields

$$\begin{aligned} u_{m+1} &= u_m + \tau \boldsymbol{b}^\top (I - z\mathbf{B})^{-1} [\lambda (u_m \boldsymbol{e} - \mathbf{\Phi}) + \dot{\mathbf{\Phi}} + \tau \boldsymbol{\gamma} (\ddot{\varphi}_m - \lambda \dot{\varphi}_m)] \\ &= u_m + z \boldsymbol{b}^\top (I - z\mathbf{B})^{-1} [u_m \boldsymbol{e} - \mathbf{\Phi} - \tau \boldsymbol{\gamma} \dot{\varphi}_m] \\ &\quad + \tau \boldsymbol{b}^\top (I - z\mathbf{B})^{-1} [\dot{\mathbf{\Phi}} + \tau \boldsymbol{\gamma} \ddot{\varphi}_m]. \end{aligned} \tag{19}$$

Theorem 5.1. *The local error of a Rosenbrock–Wanner method applied to the stiff Prothero–Robinson example (1) can be written in the case $z \to \infty$ and $\tau \to 0$ as*

$$\epsilon(t_{m+1}) = R(z)(u_m - \varphi(t_m)) + \delta_\tau(t_m), \tag{20}$$

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where

$$\delta_\tau(t_{m+1}) = \sum_{k=2}^{p} \left[\boldsymbol{b}^\top \mathbf{B}^{-1}\boldsymbol{\alpha}^k - 1\right] \varphi_m^{(k)} \frac{\tau^k}{k!} + \mathcal{O}(\tau^{p+1})$$
$$+ \sum_{k=3}^{\infty} \boldsymbol{b}^\top \sum_{l=1}^{k-2} \Big\{ \mathbf{B}^{-l-1}\left[\boldsymbol{\alpha}^{k-l} + \boldsymbol{\gamma}\delta_{k-l,1}\right] \frac{1}{(k-l)}$$
$$-\mathbf{B}^{-l}\left[\boldsymbol{\alpha}^{k-l-1} + \boldsymbol{\gamma}\delta_{k-l-1,1}\right]\Big\} \cdot \varphi_m^{(k-l)} \frac{\tau^{k-l}}{(k-l-1)! z^l}.$$

Proof. see [21]. □

This representation of the local error leads to the order conditions

$$\boldsymbol{b}^\top \mathbf{B}^{-1}\boldsymbol{\alpha}^k = 1, \quad k = 2, \dots, \bar{q}, \tag{21}$$

$$\boldsymbol{b}^\top \mathbf{B}^{-(l+1)} \frac{1}{k-l} \boldsymbol{\alpha}^{k-l} = \boldsymbol{b}^\top \mathbf{B}^{-l}\left[\boldsymbol{\alpha}^{k-l-1} + \boldsymbol{\gamma}\delta_{k-l-1,1}\right], \tag{22}$$

for $l = \max\{1, k-\bar{q}\}, \dots, k-2$ and $k = 3, \dots, \infty$. With the help of these order conditions we can formulate the next theorem and check B_{PR}-consistency.

Theorem 5.2. *A Rosenbrock–Wanner method is B_{PR}-consistent of order $\bar{q}$ if condition (21) is satisfied for $k = 2, \dots, \bar{q}$ and (22) for $k = 2, \dots, \infty$ and $l = \max\{1, k-\bar{q}\}, \dots, k-2$.*

For 2nd order Rosenbrock–Wanner methods our condition (22) for $k = l-2$ coincides with the order conditions from [13] and [24], since only equations of the form

$$\boldsymbol{b}^\top \mathbf{B}^{-(l+1)} \frac{1}{2} \boldsymbol{\alpha}^2 = \boldsymbol{b}^\top \mathbf{B}^{1-l} \boldsymbol{e}$$

are used to ensure B_{PR}-convergence of order 2.

With the help of Theorem 2.3 we have

Theorem 5.3. *A Rosenbrock–Wanner method is B_{PR}-convergent of order $\bar{q}$ if the method is A-stable with $R(\infty) < 1$ and B_{PR}-consistent of order $\bar{q}$, i.e. the global error satisfies*

$$\epsilon(t_m) \le C_1 \tau^{\bar{q}} + C_2 \frac{\tau^{\bar{q}+1}}{|z|},$$

where C_1 and C_2 are non-negative constants which are independent of τ and λ.

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This result is different from the one which is presented in a paper of Scholz (see [24]). In that paper it is formulated that every A-stable ROW method with $R(\infty) < 1$ converges with order $q+1$. This statement is in general not true, since in the proof of [24] the error constant is constructed in such way that it depends on the step-size τ. In this case an expansion gives us an expression of the form $C = \mathcal{O}(1/\tau)$, which reduces the convergence order by one. This theoretical investigation can be shown numerically, too. We will later show in our numerical results that there exists stiffly accurate ROW methods which converge with order 1 in the stiff case.

6 Results for ROW methods

6.1 Convergence analysis for 2nd order ROW methods

In the literature many 2nd order methods can be found. First we mention the ROS2 method from [28]. In this case we have $\gamma = 1 + 1/\sqrt{2}$, $\alpha_2 = 1$, $\gamma_2 = -2\gamma$, and $b_1 = b_2 = 1/2$. It is an L-stable W-method which does not satisfy equations (21) and (22). Therefore, this method is only B_{PR}-consistent of order 1. In the stiff case we have the remainders $\mathcal{O}(\tau^2)$ and $\mathcal{O}(\tau^2/z)$. The remainder $\mathcal{O}(\tau^2)$ is more dominant than $\mathcal{O}(\tau^2/z)$, since $|z|$ is large in the stiff case. Since the method is L-stable we have second order convergence in the stiff case, too.

Next we improve the ROS2 method in the following way. We skip the condition for W-methods and create a stiffly accurate method, i.e. we have $\alpha_2 = 1$. Moreover, we set again $\gamma = 1 + 1/\sqrt{2}$ and get $\beta_2 = 1 - \gamma$. We call this method ROS2SIMPLE. Now condition (21) is satisfied for all $k \geq 2$ and therefore the local error is given by $\mathcal{O}(\tau^2/z)$. In comparison with the ROS2 method we get now better results, but these results are only of first order, as we will see later.

In [24, Formula (4.5)] we find the Scholz4_5 method, which is A-stable with $R(\infty) = -1$. This method has two internal stages and we have $\gamma = 1/2$, $\alpha_2 = -\gamma_{21} = 3/4$, $b_1 = 1/9$, and $b_2 = 8/9$. This method is B_{PR}-consistent of order 2, as the following Lemma shows us.

Lemma 6.1. *The Scholz4_5 method is B_{PR}-consistent of order 2.*

Proof. First we note that $\beta_2 = \alpha_2 + \gamma_{21} = 0$. Then the matrix $\mathbf{B}$ is simply a diagonal matrix, where the diagonal entries of the inverse matrix are given by $1/\gamma$. Condition (22) for $k = 3, \ldots, \infty$ and $k - l = 2$ reads then as

$$\boldsymbol{b}^\top \mathbf{B}^{-(l+1)} \boldsymbol{\alpha}^2 = 2\boldsymbol{b}^\top \mathbf{B}^{-l+1} \boldsymbol{e}.$$

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A simple calculation gives us the condition $b_2\alpha_2^2 = 2\gamma^2$, which is fulfilled in our case, since $\gamma = 1/2$ and $b_2 = 1/(2\alpha_2^2)$. Since (21) is satisfied for $k = 2$ we have proven the B_{PR}-consistency of order 2. $\square$

Since the Scholz4_5 method is A-stable with $R(\infty) = -1$ the order of convergence is equal to the order of the local error.

The ROS2PR method from [20] is a stiffly accurate ROW method with 3 internal stages. The coefficients of the ROS2PR method are presented in Table 4. This method is not B_{PR}-consistent of order 2, since condition (22) is not satisfied for $k = 4$ and $l = 2$. For problems with medium stiffness the convergence behaviour is very poor (see [25]).

Table 4: Set of coefficients for the ROS2PR method

γ	$=$	$2.28155493653962e-01$			
α_{21}	$=$	$1.00000000000000e+00$	γ_{21}	$=$	$-2.28155493653962e-01$
α_{31}	$=$	$0.00000000000000e+00$	γ_{31}	$=$	$6.47798871261042e-01$
α_{32}	$=$	$1.00000000000000e+00$	γ_{32}	$=$	$-8.75954364915004e-01$
b_1	$=$	$6.47798871261042e-01$	$\hat{b}_1$	$=$	$7.71844506346038e-01$
b_2	$=$	$1.24045635084996e-01$	$\hat{b}_2$	$=$	$2.28155493653962e-01$
b_3	$=$	$2.28155493653962e-01$	$\hat{b}_3$	$=$	$0.00000000000000e+00$

Our last method to be considered is the stiffly accurate W-method ROS2S (see [10]) which has three internal stages. The coefficients are presented in Table 5.

Table 5: Set of coefficients for the ROS2S method

γ	$=$	$2.92893218813452e-01$			
α_{21}	$=$	$5.85786437626905e-01$	γ_{21}	$=$	$-5.85786437626905e-01$
α_{31}	$=$	$0.00000000000000e+00$	γ_{31}	$=$	$3.53553390593274e-01$
α_{32}	$=$	$1.00000000000000e+00$	γ_{32}	$=$	$-6.46446609406726e-01$
b_1	$=$	$3.53553390593274e-01$	$\hat{b}_1$	$=$	$3.33333333333333e-01$
b_2	$=$	$3.53553390593274e-01$	$\hat{b}_2$	$=$	$3.33333333333333e-01$
b_3	$=$	$2.92893218813452e-01$	$\hat{b}_3$	$=$	$3.33333333333333e-01$

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Lemma 6.2. *The ROS2S method is B_{PR}-consistent of order 2.*

Proof. We have to show that

$$\boldsymbol{b}^\top \mathbf{B}^{-l}(\mathbf{B}^{-1}\boldsymbol{\alpha}^2 - 2\mathbf{B}\boldsymbol{e}) = 0$$

is satisfied for all $l \geq 1$. The matrix $\mathbf{B}^k$, $k \geq 0$ can be inverted analytically and is given by

$$\mathbf{B}^{-k} = \frac{1}{\gamma^{k+1}} \begin{pmatrix} \gamma & 0 & 0 \\ 0 & \gamma & 0 \\ -k\beta_{31} & -k\beta_{32} & \gamma \end{pmatrix}, \qquad k \geq 0. \tag{23}$$

First we show that the vector-matrix product $\boldsymbol{b}^\top \mathbf{B}^{-l}$ is of the form (x, x, y) with $x, y \in \mathbb{R}$. In the case of ROS2S method we have $b_1 = b_2$ and $b_3 = \gamma$ (see Table 5) and get

$$\boldsymbol{b}^\top \mathbf{B}^{-l} = \left(\frac{b_1}{\gamma^l} - \gamma l \frac{b_1}{\gamma^{l+1}}, \frac{b_1}{\gamma^l} - \gamma l \frac{b_1}{\gamma^{l+1}}, \frac{1}{\gamma^{l-1}} \right).$$

Moreover, we have

$$\mathbf{B}^{-1}\boldsymbol{\alpha}^2 - 2\mathbf{B}\boldsymbol{e} = \left(-2\gamma, \frac{\alpha^2}{\gamma} - 2\gamma, -\frac{b_2\alpha_2^2}{\gamma^2} + \frac{1}{\gamma} - 2 \right)^\top.$$

Since $\alpha_2 = 2\gamma$ and $b_2\alpha_2 = 1/2 - \gamma$ it follows

$$\mathbf{B}^{-1}\boldsymbol{\alpha}^2 - 2\mathbf{B}\boldsymbol{e} = (-2\gamma, 2\gamma, 0)^\top.$$

It follows

$$\boldsymbol{b}^\top \mathbf{B}^{-l}(\mathbf{B}^{-1}\boldsymbol{\alpha}^2 - 2\mathbf{B}\boldsymbol{e}) = 0$$

and the ROS2S method is B_{PR}-consistent of order 2. □

Let us now summarise our theoretical results about the local and global errors of ROW methods. A consistent ROW method has the local error $\mathcal{O}(\tau^2)$, if no further order conditions are satisfied and the method is not stiffly accurate. In this case the method converges with order 2 in the stiff case. The disadvantage of this method is the relatively large error constant. This error constant can be reduced if the method was stiffly accurate. But in this case now the local error is given by $\mathcal{O}(\tau^2/z)$, i.e. the method converges only with order 1. This convergence behaviour can be improved if the method would fulfil condition (22) for certain k and l.

The properties of the studied methods are presented in Table 6. Moreover, we check whether the order conditions (21) (see column 6 and 7) and (22) (see columns 8, 9 and 10) are fulfilled.

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Table 6: Properties of selected 2nd order ROW methods

method	s	p	stiffly acc	$R(\infty)$	2	3	$k=3$ $l=1$	4 2	4 1
ROS2	2	2	-	0	-	-	-	-	-
ROS2SIMPLE	2	2	x	0	x	x	-	-	-
ROS2S	3	2	x	0	x	x	x	x	-
ROS2PR	3	2	x	0	x	x	x	-	-
Scholz4_5	2	2	-	-1	x	-	x	x	-

6.2 Numerical results for 2nd order ROW methods

Next we solve the example of Prothero–Robinson example (1), where the function $\varphi(t)$ is given by

$$\varphi(t) = 10 - (10 + t)\exp(-t).$$

We solve this problem in the time interval $[0, 2]$ and use the same setting as in Section 4.2. In Figure 4 we present the numerical results. In the left part the results for medium stiffness $\lambda = -10^3$ are shown. Since the ROS2 method does not satisfy any further order conditions the numerical results are rather poor, but of order 2. The results for the ROS2SIMPLE method are better than those of the ROS2 method if τ is large, otherwise both methods compute similar solutions. The ROS2PR method satisfies only condition (22) for $k = 3$ and $l = 1$. This has the effect that the convergence order is small and the numerical results are not satisfactory. For this experiment the remainder $\mathcal{O}(\tau^2/z^2)$ dominates the error if larger step-sizes are used. The Scholz4_5 method converges for large τ with order 3, but the best results for all step-sizes τ are obtained by the ROS2S method, since this method is B_{PR}-consistent of order 2.

Next we consider the results for the stiff case, i.e. $\lambda = -10^6$. Here we get different results. First we observe that the ROS2 method delivers the poorest results, but again the numerical results are of second order. Better results are obtained with the ROS2SIMPLE method, but the method converges only with order 1, since the method is stiffly accurate. The Scholz4_5 method has again the highest convergence order, i.e. order 3, but the numerical results are not the best ones. In this case the ROS2PR and ROS2S methods give the best results. In the case of the ROS2PR method we observe convergence order 2 for larger step-sizes and almost no convergence for smaller step-sizes, i.e. the numerical error stagnates at 10^{-11}. This is the same problem as for

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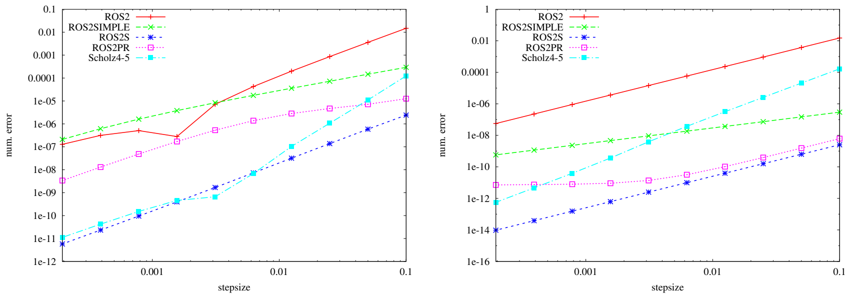

Figure 4: τ versus error for (1) with $\lambda = -10^3$ (left) and $\lambda = -10^6$ (right)

the SDIRK2PR method, since the error is dominated for smaller step-sizes by the term $\mathcal{O}(\tau^2/z^2)$.

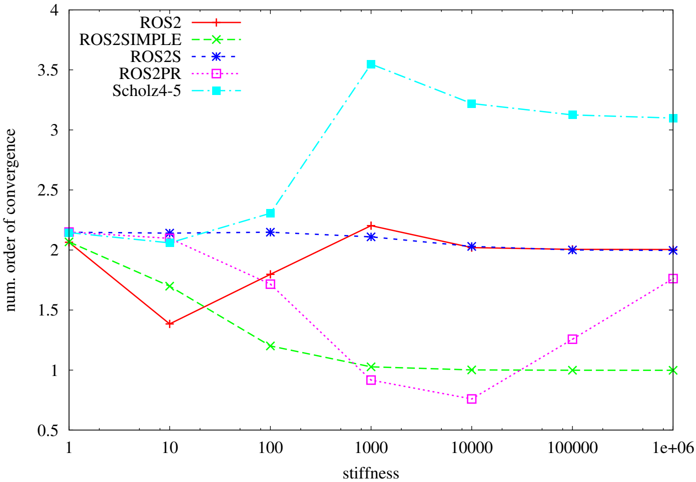

Figure 5: λ versus numerical order of convergence for (1)

In Figure 5 we plot the stiffness factor $|\lambda|$ against the numerical order of convergence. The ROS2 method converges more or less with order 2 for all λ. For $\lambda = -10$ the numerical convergence order decreases. The reason for this behaviour might be that now the remainder $\mathcal{O}(\tau^2/z)$ comes into play. For the ROS2SIMPLE method the order of convergence decreases from 2 for non-stiff problems to 1 for stiff problems. As mentioned above the numerical

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convergence order for medium stiff λ is rather poor for the ROS2PR method, since different remainders become dominant. The ROS2S method converges, with order 2 for all λ, since the method is B_{PR}-consistent of order 2. The Scholz4_5 method shows an interesting result. For small λ, i.e. for non-stiff problems, the method converges with order 2, since only the 2nd order conditions are satisfied. If the problem becomes stiff order 3 can be archived, since the local error is bounded by $\mathcal{O}(\tau^3)$.

Finally the numerical error is plotted for very small step-sizes τ to show that for all methods the numerical error can be reduced to machine accuracy. We solve the Prothero–Robinson example with $\lambda = -10^6$ and use the step-sizes $\tau = 1/(100 \cdot 2^k)$ with $k = 0, \ldots, 11$. The results are plotted in

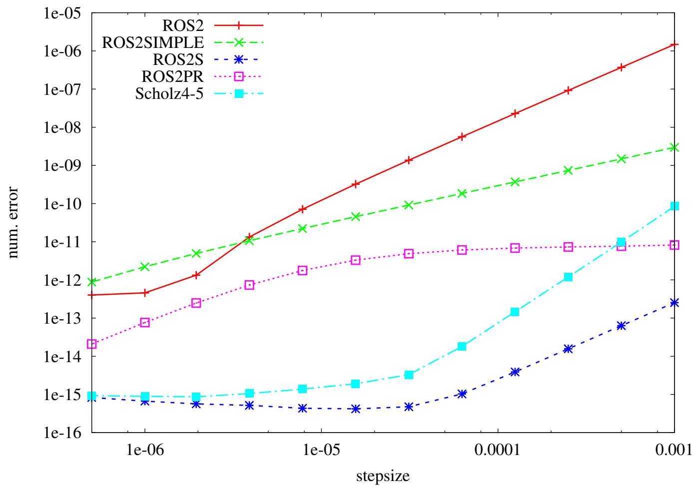

Figure 6: τ versus numerical error for (1) with $\lambda = -10^6$

Figure 6. The ROS2 method converges with order 2 for larger step-sizes, and for smaller ones the convergence order decreases. The ROS2SIMPLE method converges with order 1. For smaller step-sizes the order increases. In comparison to the ROS2 method it can observed that the ROS2SIMPLE method gives more accurate results for larger time step-sizes than the ROS2 method. The ROS2PR method converges with 2nd order only for small step-sizes, but the numerical results are more accurate for all step-sizes than the numerical results of the ROS2 and the ROS2SIMPLE method. The Scholz4_7 method has convergence order 3, and in this example the numerical results are more accurate than the ones of ROS2, ROS2SIMPLE and ROS2PR. The

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best results are obtained with the ROS2S method, since it is B_{PR}-consistent of order 2.

6.3 Convergence analysis for ROW Methods of order 3

Before we discuss the B_{PR}-consistency of existing ROW methods we start our considerations with some results.

Lemma 6.3. *Consider a Rosenbrock–Wanner method of order 3 with 3 internal stages which satisfies the following conditions:*

$$\beta_2 = 0, \qquad \gamma^2 - \gamma + 1/6 = 0, \qquad b_3\beta_{32}\alpha_2^2 = \gamma/6 - \gamma^3.$$

Then the method is B_{PR}-consistent of order 2.

Proof. We have to show that

$$\boldsymbol{b}^\top \mathbf{B}^{-l}(\mathbf{B}^{-1}\boldsymbol{\alpha}^2 - 2\mathbf{B}\boldsymbol{e}) = 0$$

is satisfied for all $l \geq 1$. Using the representation of $\mathbf{B}^{-l}$, i.e. equation (23), we get

$$\begin{aligned}\boldsymbol{b}^\top \mathbf{B}^{-l}(\mathbf{B}^{-1}\boldsymbol{\alpha}^2 - 2\mathbf{B}\boldsymbol{e}) &= \frac{1}{\gamma^{l+1}}(b_2\alpha_2^2 + b_3\alpha_3^2) - \frac{l+1}{\gamma^{l+2}}b_3\beta_{32}\alpha_2^2 \\ &\quad - \frac{2}{\gamma^{l-1}}(b_1 + b_2 + b_3) + \frac{2}{\gamma^l}(l-1)b_3\beta_3.\end{aligned}$$

Next we insert the order conditions for ODEs up to order 3 and get

$$\begin{aligned}&\boldsymbol{b}^\top \mathbf{B}^{-l}(\mathbf{B}^{-1}\boldsymbol{\alpha}^2 - 2\mathbf{B}\boldsymbol{e}) \\ &\qquad = \frac{1}{3\gamma^{l+1}} - \frac{l+1}{\gamma^{l+2}}b_3\beta_{32}\alpha_2^2 - \frac{2}{\gamma^{l-1}} + \frac{1}{\gamma^l}(l-1)(1-2\gamma).\end{aligned}$$

Next we use the assumption $b_3\beta_{32}\alpha_2^2 = \gamma/6 - \gamma^3$ and get

$$\begin{aligned}&\boldsymbol{b}^\top \mathbf{B}^{-l}(\mathbf{B}^{-1}\boldsymbol{\alpha}^2 - 2\mathbf{B}\boldsymbol{e}) \\ &\qquad = \frac{1}{\gamma^{l+1}}\left(\frac{1}{3} - \frac{l+1}{6}(1-6\gamma^2) - 2\gamma^2 + \gamma(l-1)(1-2\gamma)\right) = 0,\end{aligned}$$

since $\gamma^2 - \gamma + 1/6 = 0$. □

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Lemma 6.4. *The order condition (22) for $k = 3, \ldots, \infty$ and $k - l = 3$ is satisfied if the coefficients are chosen by*

$$\alpha_2 = 3\gamma, \tag{24}$$

$$\sum_{j=2}^{s-1} \beta_{ij}\alpha_j^2 + \gamma\alpha_i^2 = \alpha_i^3/3, \qquad i = 3, \ldots, s. \tag{25}$$

Proof. Condition (22) for $k = 3, \ldots, \infty$ and $k - l = 3$ reads as

$$\boldsymbol{b}^\top \mathbf{B}^{-(l+1)} \left(\boldsymbol{\alpha}^3 - 3\mathbf{B}\boldsymbol{\alpha}^2\right).$$

This equation is satisfied if $3\mathbf{B}\boldsymbol{\alpha}^2 = \boldsymbol{\alpha}^3$ holds, and thus the Theorem is proven. $\square$

In the literature many third order methods can be found. Here we consider only methods, which satisfy further order conditions to improve the numerical order of convergence. From [12] we have the ROS3P method which is strongly A-stable and has three internal stages. Table 7 presents the coefficients of the method. The ROS3P method is only B_{PR}-consistent of order 2, as the

Table 7: Set of coefficients for the ROS3P method

γ	$=$	$7.88675134594813e-01$			
α_{21}	$=$	$1.00000000000000e+00$	γ_{21}	$=$	$-1.00000000000000e+00$
α_{31}	$=$	$1.00000000000000e+00$	γ_{31}	$=$	$-7.88675134594813e-01$
α_{32}	$=$	$0.00000000000000e+00$	γ_{32}	$=$	$-1.07735026918963e+00$
b_1	$=$	$6.66666666666667e-01$	$\hat{b}_1$	$=$	$3.33333333333333e-01$
b_2	$=$	$0.00000000000000e+00$	$\hat{b}_2$	$=$	$3.33333333333333e-01$
b_3	$=$	$3.33333333333333e-01$	$\hat{b}_3$	$=$	$3.33333333333333e-01$

following Lemma states.

Lemma 6.5. *The ROS3P method is B_{PR}-consistent of order 2.*

Proof. The coefficients of the ROS3P method fulfil $\beta_2 = 0$ and $\gamma^2 - \gamma + 1/6 = 0$. It remains to show that $b_3\beta_{32}\alpha_2^2 = \gamma/6 - \gamma^3$ holds. With the investigations from Lang and Verwer [12] we show that

$$b_3\beta_{32}\alpha_2^2 = \frac{1/2 - \gamma}{\beta_3} \cdot \frac{(1 - 4\gamma)}{6(1/2 - \gamma)\alpha_2^2}\beta_3\alpha_2^2 = \frac{1 - 4\gamma}{6}$$

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holds. Since $\gamma = \frac{1}{2}\left(1+1/\sqrt{3}\right)$ we have $b_3\beta_{32}\alpha_2^2 = \gamma/6 - \gamma^3$, and the ROS3P method is B_{PR}-consistent of order 2. Moreover, condition (21) is satisfied for all $k \geq 2$, since

$$\boldsymbol{b}^\top \mathbf{B}^{-1}\boldsymbol{\alpha}^k = \frac{1}{\gamma^2}\left(\gamma b_2\alpha_2^k - b_3\beta_{32}\alpha_2^k + \gamma b_3\alpha_3^k\right).$$

With the setting $\alpha_2 = \alpha_3 = 1$ the order conditions reduce to $b_2 + b_3 = 1/3$ and $b_3\beta_{32} = \gamma/3 - \gamma^2$ and, finally we have $\boldsymbol{b}^\top \mathbf{B}^{-1}\boldsymbol{\alpha}^k = 1$ for all $k \geq 2$. $\square$

Lemma 6.5 implies that the local error of the method is given by $\mathcal{O}(\tau^3/z)$. Since $R(\infty) \approx -0.73$ the global error of ROS3P is of order τ^3/z, too.

In the paper of Scholz [24, Formula (4.7)] we can find the method Scholz4_7, where the coefficient α_3 is a free variable. If $\alpha_3 = 1$ we get the method ROS3PR, which can be found in [22], too. This method has three internal stages and is strongly A-stable. The coefficients of ROS3PR are presented in Table 8. In [24, Formula (4.7)] a second method with $\alpha_3 = 5/4$ is

Table 8: Set of coefficients for the ROS3PR method .

γ	=	$7.88675134594813e-01$			
α_{21}	=	$2.36602540378444e+00$	γ_{21}	=	$-2.36602540378444e+00$
α_{31}	=	$0.00000000000000e+00$	γ_{31}	=	$-2.84686425165674e-01$
α_{32}	=	$1.00000000000000e+00$	γ_{32}	=	$-1.08133897861876e+00$
b_1	=	$2.92663844023951e-01$	$\hat{b}_1$	=	$1.11324865405187e-01$
b_2	=	$-8.13389786187641e-02$	$\hat{b}_2$	=	$1.00000000000000e-01$
b_3	=	$7.88675134594813e-01$	$\hat{b}_3$	=	$7.88675134594813e-01$

considered. This method is denoted by Scholz4_7B, and the coefficients can be found in Table 9.

Lemma 6.6. *The ROS3PR and Scholz4_7B methods are B_{PR}-consistent of order 3.*

Proof. Let us first consider the ROS3PR method. The method satisfies the assumptions of Lemma 6.3. Therefore, the ROS3PR is at least B_{PR}-consistent of order 2. Next we check the assumptions of Lemma 6.4. We have only to check assumption (25), since $\alpha_2 = 3\gamma$. Condition (25) reads as

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Table 9: Set of coefficients for the SCHOLZ4_7 method

γ	$=$	$7.88675134594813e-01$			
α_{21}	$=$	$2.36602540378444e+00$	γ_{21}	$=$	$-2.36602540378444e+00$
α_{31}	$=$	$2.50000000000000e-01$	γ_{31}	$=$	$-6.13414364537605e-01$
α_{32}	$=$	$1.00000000000000e+00$	γ_{32}	$=$	$-1.10383267558217e+00$
b_1	$=$	$4.95076910424059e-01$	$\hat{b}_1$	$=$	$3.33333333333333e-01$
b_2	$=$	$-1.12898126628685e-01$	$\hat{b}_2$	$=$	$3.33333333333333e-01$
b_3	$=$	$6.17821216204626e-01$	$\hat{b}_3$	$=$	$3.33333333333333e-01$

$9\beta_{32}\gamma^2+\gamma = 1/3$, which is in our case satisfied, since $\beta_{32} = -(8+\sqrt{3})/9$. Condition (21) is satisfied for all $k \geq 2$. Therefore, the method is B_{PR}-consistent of order 3.

The B_{PR}-consistency of the Scholz4_7B method can be proven in an analogous way. In this case condition (21) is only satisfied for $k = 3$. $\square$

In the case of the Scholz4_7B method the local error is dominated in the stiff case $\mathcal{O}(\tau^3)$. Since the method is strongly A-stable with $R(\infty) = -0.73$ the global error is equal to the local error if equidistant time-steps are used. In contrast to the Scholz4_7B method the local and global error of the ROS3PR method are given by $\mathcal{O}(\tau^4/z)$.

Next we discuss stiffly accurate ROW methods with 4 internal stages. All methods are stiffly accurate, i.e. equation (21) is satisfied for all $k \geq 2$. Then we can prove the following Lemma.

Lemma 6.7. *Let a stiffly accurate ROW method be given which satisfies the conditions*

$$\beta_2 = 0 \qquad \textit{and} \qquad b_3\beta_{32}\alpha_2^2 = 2\gamma^3 - 2\gamma^2 + \frac{1}{3}\gamma. \tag{26}$$

Then the method is B_{PR}-consistent of order 2.

Proof. We have to show that

$$\boldsymbol{b}^\top \mathbf{B}^{-l}(\mathbf{B}^{-1}\boldsymbol{\alpha}^2 - 2\mathbf{B}\boldsymbol{e}) = 0, \qquad \text{for all } l \geq 1.$$

Therefore, we first compute potentials of the inverse of $\mathbf{B}$ which are given in

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general by

$$\mathbf{B}^{-l} = \begin{pmatrix} \frac{1}{\gamma^l} & 0 & 0 & 0 \\ 0 & \frac{1}{\gamma^l} & 0 & 0 \\ \frac{-l\beta_{31}}{\gamma^{l+1}} & \frac{-l\beta_{32}}{\gamma^{l+1}} & \frac{1}{\gamma^l} & 0 \\ \frac{-(\eta(l)b_3\beta_{31}+\gamma l b_1)}{\gamma^{l+2}} & \frac{-(\eta(l)b_3\beta_{32}+\gamma l b_2)}{\gamma^{l+2}} & \frac{-lb_3}{\gamma^{l+1}} & \frac{1}{\gamma^l} \end{pmatrix},$$

where $\eta(l)$ is some constant in dependency of the potential l. Moreover, we have

$$\begin{aligned} \mathbf{B}^{-1}\boldsymbol{\alpha}^2 - 2\mathbf{B}\boldsymbol{e} = -2 \begin{pmatrix} \gamma \\ \gamma \\ \beta_3 + \gamma \\ 1 \end{pmatrix} + \frac{1}{\gamma} \begin{pmatrix} 0 \\ \alpha_2^2 \\ \alpha_3^2 \\ 1 \end{pmatrix} \\ - \frac{1}{\gamma^2} \begin{pmatrix} 0 \\ 0 \\ \beta_{32}\alpha_2^2 \\ \beta_3\alpha_3^2 \end{pmatrix} + \frac{1}{\gamma^3} \begin{pmatrix} 0 \\ 0 \\ 0 \\ (b_3\beta_{32} - b_2\gamma)\alpha_2^2 \end{pmatrix}. \end{aligned}$$

Then it follows

$$\boldsymbol{b}^\top \mathbf{B}^{-l-1}(\mathbf{B}^{-1}\boldsymbol{\alpha}^2 - 2\mathbf{B}\boldsymbol{e}) = (0,0,0,1)\mathbf{B}^{-l}(\mathbf{B}^{-1}\boldsymbol{\alpha}^2 - 2\mathbf{B}\boldsymbol{e}),$$

since the method is stiffly accurate. Next we insert the results from above and get

$$\begin{aligned} \gamma^{l+2}(0,0,0,1)\mathbf{B}^{-l}(\mathbf{B}^{-1}\boldsymbol{\alpha}^2 - 2\mathbf{B}\boldsymbol{e}) &= 2\gamma(\eta(l)b_3\beta_{31} + \gamma l b_1) \\ &\quad - (\eta(l)b_3\beta_{32} + \gamma l b_2)(-2\gamma + \alpha_2^2/\gamma) \\ &\quad - lb_3(-2\gamma(\beta_3 + \gamma) + \alpha_3^2 - \beta_{32}\alpha_2^2/\gamma) \\ &\quad - 2\gamma^2 + \gamma - b_3\alpha_3^2 + (b_3\beta_{32} - b_2\gamma)\alpha_2^2/\gamma. \end{aligned}$$

First we collect all the terms which depend on $\eta(l)$ and get

$$\begin{aligned} &2\gamma b_3(\beta_{31} + \beta_{32}) - b_3\beta_{32}\alpha_2^2/\gamma \\ &\quad = 2\gamma(1/2 - 2\gamma + \gamma^2) - (2\gamma^2 - 2\gamma + 1/3) = 2\gamma^3 - 6\gamma^2 + 3\gamma - 1/3 = 0, \end{aligned}$$

since the method is L-stable. Next we collect the remaining terms which depend on l. We have

$$2\gamma^2(b_1 + b_2 + b_3) - (b_2\alpha_2^2 + b_3\alpha_3^2) + b_3\beta_{32}\alpha_2^2/\gamma + 2\gamma b_3\beta_3 = 0,$$

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since the method satisfies the conditions for order 3. For the remaining terms we have

$$-2\gamma^2 + \gamma - (b2\alpha_2^2 + b_3\alpha_3^2) + b_3\beta_{32}\alpha_2^2/\gamma = 0.$$

Therefore, it follows

$$\gamma^{l+2}(0,0,0,1)\mathbf{B}^{-l}(\mathbf{B}^{-1}\boldsymbol{\alpha}^2 - 2\mathbf{B}\boldsymbol{e}) = 0$$

and the method is B_{PR}-consistent of order 2. □

In the paper of Lang and Teleaga [11] the ROS3PL method can be found, which has 4 internal stages and is stiffly accurate. For the coefficients we refer to Table 10. This method is B_{PR}-consistent of order 2, since the assumptions of Lemma 6.7 are satisfied. But the method does not satisfy the new order condition (22) for $k = 4$ and $l = 1$ (see also Table 14).

Table 10: Set of coefficients for the ROS3PL method

γ	$=$	$4.35866521508459e-01$			
α_{21}	$=$	$5.00000000000000e-01$	γ_{21}	$=$	$-5.00000000000000e-01$
α_{31}	$=$	$5.00000000000000e-01$	γ_{31}	$=$	$-8.50974004860610e-01$
α_{32}	$=$	$5.00000000000000e-01$	γ_{32}	$=$	$5.261356558646561e-01$
α_{41}	$=$	$5.00000000000000e-01$	γ_{41}	$=$	$-3.33333333333333e-01$
α_{42}	$=$	$5.00000000000000e-01$	γ_{42}	$=$	$1.66666666666667e-01$
α_{43}	$=$	$0.00000000000000e+00$	γ_{43}	$=$	$-2.69199854841792e-01$
b_1	$=$	$1.66666666666667e-01$	$\hat{b}_1$	$=$	$5.00000000000000e-01$
b_2	$=$	$6.66666666666667e-01$	$\hat{b}_2$	$=$	$3.52063575111237e-01$
b_3	$=$	$-2.69199854841792e-01$	$\hat{b}_3$	$=$	$-1.74031608728707e-01$
b_4	$=$	$4.35866521508459e-01$	$\hat{b}_4$	$=$	$3.21968033617470e-01$

Then we consider the W-method ROS34PW2 from [23]. The method is B_{PR}-consistent of order 2, because the assumptions of Lemma 6.7 are fulfilled. This method does not satisfy the new order condition (22) for $k = 4$ and $l = 1$, either, (see also Table 14).

An extension of the the ROS34PW2 method is the method ROS34PRW (see [19]). This method satisfies the new order condition (22) for $k = 4$ and $l = 1$, but not for $k = 5$ and $l = 2$ (see also Table 14). Therefore, this method is only B_{PR}-consistent of order 2, too. The numerical error is of order $\mathcal{O}(\tau^4/z) + \mathcal{O}(\tau^3/z^2)$, which has the effect that the convergence decreases for median stiff problems. The coefficients are displayed in Table 12.

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Table 11: Set of coefficients for ROS34PW2

γ	$=$	$4.3586652150845900e-01$			
α_{21}	$=$	$8.7173304301691801e-01$	γ_{21}	$=$	$-8.7173304301691801e-01$
α_{31}	$=$	$8.4457060015369423e-01$	γ_{31}	$=$	$-9.0338057013044082e-01$
α_{32}	$=$	$-1.1299064236484185e-01$	γ_{32}	$=$	$5.4180672388095326e-02$
α_{41}	$=$	$0.0000000000000000e+00$	γ_{41}	$=$	$2.4212380706095346e-01$
α_{42}	$=$	$0.0000000000000000e+00$	γ_{42}	$=$	$-1.2232505839045147e+00$
α_{43}	$=$	$1.0000000000000000e+00$	γ_{43}	$=$	$5.4526025533510214e-01$
b_1	$=$	$2.4212380706095346e-01$	$\hat{b}_1$	$=$	$3.7810903145819369e-01$
b_2	$=$	$-1.2232505839045147e+00$	$\hat{b}_2$	$=$	$-9.6042292212423178e-02$
b_3	$=$	$1.5452602553351020e+00$	$\hat{b}_3$	$=$	$5.0000000000000000e-01$
b_4	$=$	$4.3586652150845900e-01$	$\hat{b}_4$	$=$	$2.1793326075422950e-01$

Table 12: Set of coefficients for the ROS34PRW method

γ	$=$	$4.35866521508459e-01$			
α_{21}	$=$	$1.30759956452538e+00$	γ_{21}	$=$	$-1.30759956452538e+00$
α_{31}	$=$	$1.4570method6112093338e+00$	γ_{31}	$=$	$-1.62236977749782e+00$
α_{32}	$=$	$-3.45563059308181e-01$	γ_{32}	$=$	$2.98332014575486e-01$
α_{41}	$=$	$-5.34022078494429e-02$	γ_{41}	$=$	$4.40241527882008e-01$
α_{42}	$=$	$5.00000000000000e-01$	γ_{42}	$=$	$-1.17785627854546e+00$
α_{43}	$=$	$5.5340method2207849443e-01$	γ_{43}	$=$	$3.01748229154996e-01$
b_1	$=$	$3.86839320032565e-01$	$\hat{b}_1$	$=$	$5.86431178611326e-01$
b_2	$=$	$-6.77856278545464e-01$	$\hat{b}_2$	$=$	$-4.61234600436573e-01$
b_3	$=$	$8.55150437004439e-01$	$\hat{b}_3$	$=$	$5.52835388207777e-01$
b_4	$=$	$4.35866521508459e-01$	$\hat{b}_4$	$=$	$3.21968033617470e-01$

An improvement of the ROS3PL method can, for example, be found in [25] and is called ROS3PRL. As the ROS34PRW method the ROS3PRL method only satisfies the new order condition (22) for $k = 4$ and $l = 1$, but not for $k = 4$ and $l = 2$ (see also Table 14). Therefore, this method is only B_{PR}-consistent of order 2. The coefficients are displayed in Table 13.

In Table 14 we display the properties of the selected methods. It can

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Table 13: Set of coefficients for the ROS3PRL method

γ	$=$	$4.35866521508459e-01$			
α_{21}	$=$	$5.00000000000000e-01$	γ_{21}	$=$	$-5.00000000000000e-01$
α_{31}	$=$	$5.00000000000000e-01$	γ_{31}	$=$	$-7.91564804204642e-01$
α_{32}	$=$	$5.00000000000000e-01$	γ_{32}	$=$	$3.52442167927514e-01$
α_{41}	$=$	$5.00000000000000e-01$	γ_{41}	$=$	$-4.97889699145187e-01$
α_{42}	$=$	$5.00000000000000e-01$	γ_{42}	$=$	$3.86075154415805e-01$
α_{43}	$=$	$0.00000000000000e+00$	γ_{43}	$=$	$-3.24051976779077e-01$
b_1	$=$	$2.11030085481324e-03$	$\hat{b}_1$	$=$	$5.00000000000000e-01$
b_2	$=$	$8.86075154415805e-01$	$\hat{b}_2$	$=$	$3.87524229532982e-01$
b_3	$=$	$-3.24051976779077e-01$	$\hat{b}_3$	$=$	$-2.09492263150452e-01$
b_4	$=$	$4.35866521508459e-01$	$\hat{b}_4$	$=$	$3.21968033617470e-01$

Table 14: Properties of selected third order ROW methods

method	s	p	stiffly acc.	$R(\infty)$	3	4	5	$k=4$ $l=2$	5 3	4 1	5 2	6 1
ROS3P	3	3	-	-0.73	x	x	x	x	x	-	-	-
ROS3PR	3	3	-	-0.73	x	x	x	x	x	x	x	-
Scholz4_7B	3	3	-	-0.73	x	-	-	x	x	x	x	-
ROS3PL	4	3	x	0.00	x	x	x	x	x	-	-	-
ROS34PW2	4	3	x	0.00	x	x	x	x	x	-	-	-
ROS34PRW	4	3	x	0.00	x	x	x	x	x	x	-	-
ROS3PRL	4	3	x	0.00	x	x	x	x	x	x	-	-

be observed that only the Scholz4_7B and the ROS3PR method satisfy condition (22) for $k = 5$ and $l = 2$. Therefore, all other methods are not B_{PR}-consistent of order 3 and thus have order reduction for the example of Prothero and Robinson.

6.4 A stiffly accurate ROW method with B_{PR}-consistency order 3

Since none of the stiffly accurate ROW methods in Table 14 is B_{PR}-consistent of order 3 we develop a method in the following. We know from existing

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methods that $\beta_2 = 0$ holds. Then the order conditions for ODEs read as

$$b_1 + b_2 + b_3 = 1 - \gamma, \tag{27}$$

$$b_3\beta_3 = \frac{1}{2} - 2\gamma + \gamma^2, \tag{28}$$

$$b_2\alpha_2^2 + b_3\alpha_3^2 = \frac{1}{3} - \gamma, \tag{29}$$

$$\frac{1}{6} - \frac{3}{2}\gamma + 3\gamma^2 - \gamma^3 = 0. \tag{30}$$

For B_{PR}-consistency of order 2 we have the order condition (26), i.e.

$$b_3\beta_{32}\alpha_2^2 = 2\gamma^3 - 2\gamma^2 + \frac{1}{3}\gamma. \tag{31}$$

Lemma 6.4 gives us the conditions for B_{PR}-consistency of order 3, i.e. $\alpha_2 = 3\gamma$ and

$$3(\beta_{32}\alpha_2^2 + \gamma\alpha_3^2) = \alpha_3^3. \tag{32}$$

From (30) we get a cubic equation for γ, i. e.

$$\gamma^3 - 3\gamma^2 + \frac{3}{2}\gamma - \frac{1}{6} = 0.$$

One solution of this equation is $\gamma \approx 0.43$. Next we express the variables in dependency of γ and α_3. The variable α_3 is a free variable. With the help of equation (32) we can determine β_{32}, i.e.

$$\beta_{32} = \alpha_3^2\frac{\alpha_3 - 3\gamma}{27\gamma^2}.$$

It follows with (31) that

$$b_3 = \gamma\frac{6\gamma^2 - 6\gamma + 1}{\alpha_3^2(\alpha_3 - 3\gamma)}$$

holds. With this information the remaining coefficients can be computed, where we use equations (27) (for b_1), (28) (for β_3), and (30) (for b_2). The embedded method should be of order 2 and strongly A-stable with $\hat{R}(\infty) = -1/4$. In this case $\hat{b}_1$ is a free variable and we set $\hat{b}_1 = 1/2$. The conditions read as

$$\hat{b}_2 + \hat{b}_3 + \hat{b}_4 = 1/2,$$

$$\hat{b}_3\beta_3 + \hat{b}_4(1-\gamma) = 1/2 - \gamma,$$

$$0 = -5\gamma^4 + 4\gamma^3 + 4\hat{b}_4\gamma^3 - 4\hat{b}_3\gamma^2\beta_3 + 4\hat{b}_4\beta_3\gamma b_3 - 4\hat{b}_4\gamma^2,$$

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which lead to the following setting of the coefficients:

$$\hat{b}_2 \approx -0.2573, \quad \hat{b}_3 \approx 0.43542, \quad \hat{b}_4 = 0.32197.$$

We present the coefficients of the ROS3PRL2 method in Table 15.

Table 15: Set of coefficients for the ROS3PRL2 method

γ	$=$	$4.35866521508459e-01$			
α_{21}	$=$	$1.30759956452538e+00$	γ_{21}	$=$	$-1.30759956452538e+00$
α_{31}	$=$	$5.00000000000000e-01$	γ_{31}	$=$	$-7.09885758609722e-01$
α_{32}	$=$	$5.00000000000000e-01$	γ_{32}	$=$	$-5.59967359602778e-01$
α_{41}	$=$	$5.00000000000000e-01$	γ_{41}	$=$	$-1.55508568075521e-01$
α_{42}	$=$	$5.00000000000000e-01$	γ_{42}	$=$	$-9.53885165751122e-01$
α_{43}	$=$	$0.00000000000000e+00$	γ_{43}	$=$	$6.73527212318184e-01$
b_1	$=$	$3.44491431924479e-01$	$\hat{b}_1$	$=$	$5.00000000000000e-01$
b_2	$=$	$-4.53885165751122e-01$	$\hat{b}_2$	$=$	$-2.57388120865221e-01$
b_3	$=$	$6.73527212318184e-01$	$\hat{b}_3$	$=$	$4.35420087247750e-01$
b_4	$=$	$4.35866521508459e-01$	$\hat{b}_4$	$=$	$3.21968033617470e-01$

6.5 Numerical results for 3rd order ROW methods

Next we compare the theoretical results with the the numerical ones and consider the Prothero–Robinson example (1) with

$$\varphi(t) = 10 - (10 + t)\exp(-t),$$

where we use the same setting as in Section 4.2. In the left part of Figure 7 we consider the medium stiffness, i.e. $\lambda = -10^3$. In this case the ROS3PR and the ROS3PRL2 methods compute the most accurate results for all step-sizes, since the methods are B_{PR}-consistent of order 3. The results of the Scholz4_7B method are for small step-sizes of the same precision as the results of ROS3PR and ROS3PRL2, but for large step-sizes the results are more inaccurate. The numerical errors of ROS3P, ROS3PL, and ROS34PW2 are the largest ones. Better results are obtained with ROS34PRW and ROS3PRL, although the numerical order of convergence decreases for large step-sizes.

In the stiff case (right part of Figure 7) we get a different impression. Again the results of ROS3P, ROS3PL, and ROS34PW2 are poor. Better

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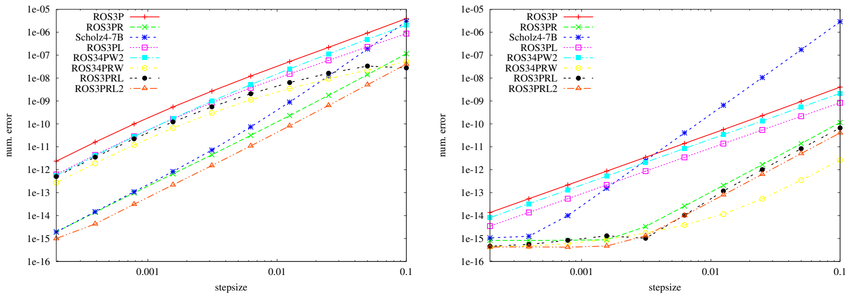

Figure 7: τ versus error for (1) with $\lambda = -10^3$ (left) and $\lambda = -10^6$ (right)

results are obtained with the ROS3PR, ROS3PRL and ROS3PRL2 methods, which in this case converge with order 3. The best results are produced by the ROS34PRL method. The highest order of convergence is obtained with the Scholz4_7B method, but the accuracy of the method is poor.

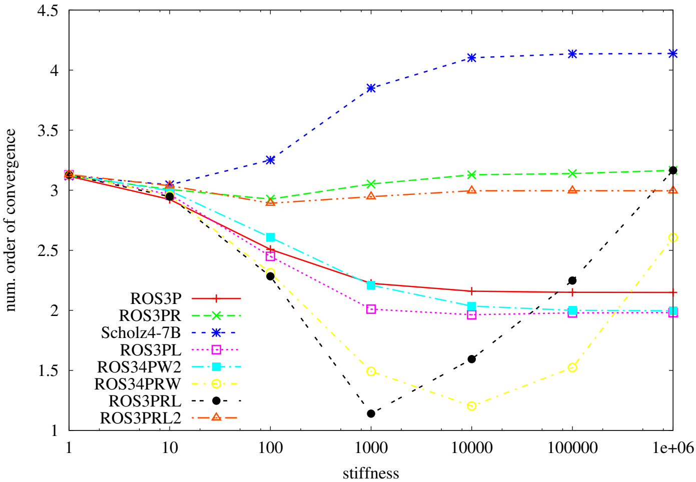

Figure 8: λ versus numerical order of convergence for (1)

In Figure 8 we plot the stiffness factor $|\lambda|$ against the numerical order of convergence. The methods ROS3P, ROS3PL, and ROS34PW2 converge with order 3 for non-stiff problems and with order 2 for stiff problems. ROS34PRW and ROS3PRL have problems with the convergence order if medium stiff

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problems are considered, since the remainder $\mathcal{O}(\tau^3/z^2)$ becomes dominant. The method ROS3PR converges with order 3 for all λ, and the Scholz4_7B method with order 4 in the stiff case.

7 Summary and Outlook

In this paper we applied Runge–Kutta and Rosenbrock–Wanner methods on the ODE of Prothero and Robinson and analysed the local and global errors. We obtained new order conditions which enabled us to construct B_{PR}-convergent methods. Numerical experiments confirm the theoretical investigations.

In further investigations other problems should be considered as, for examples, DAEs or PDEs. Moreover, other Rosenbrock–Wanner over Runge–Kutta methods can be improved.

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